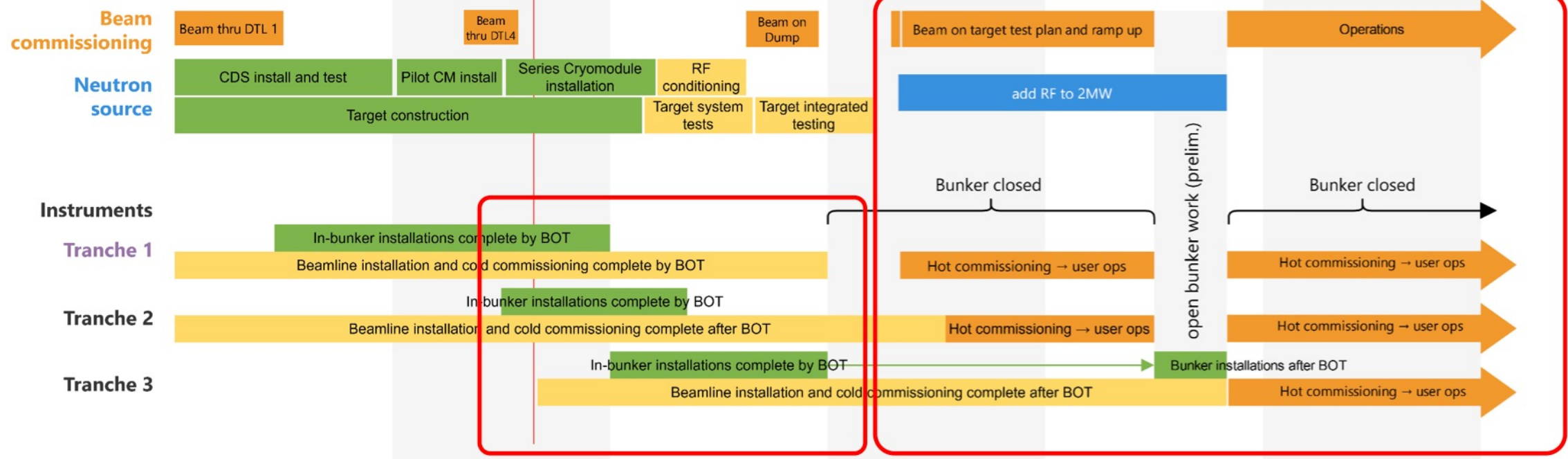
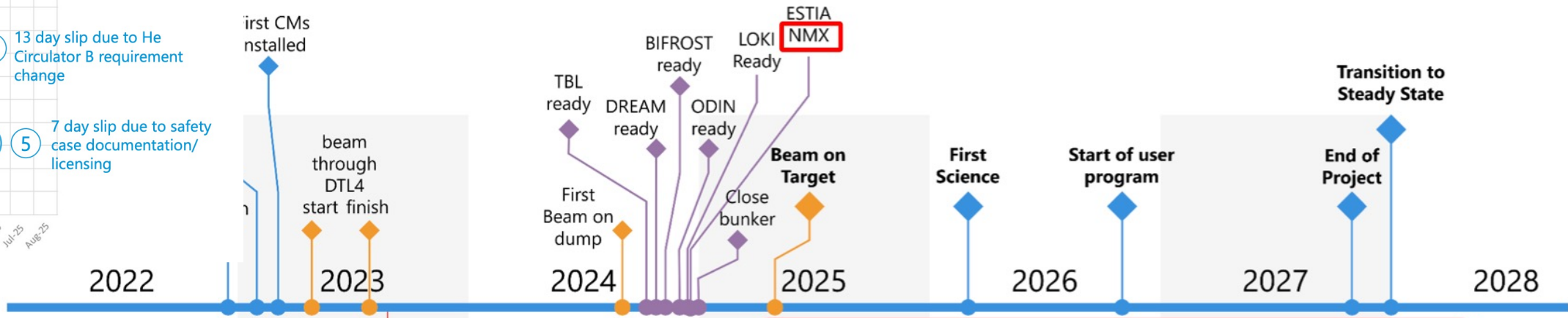
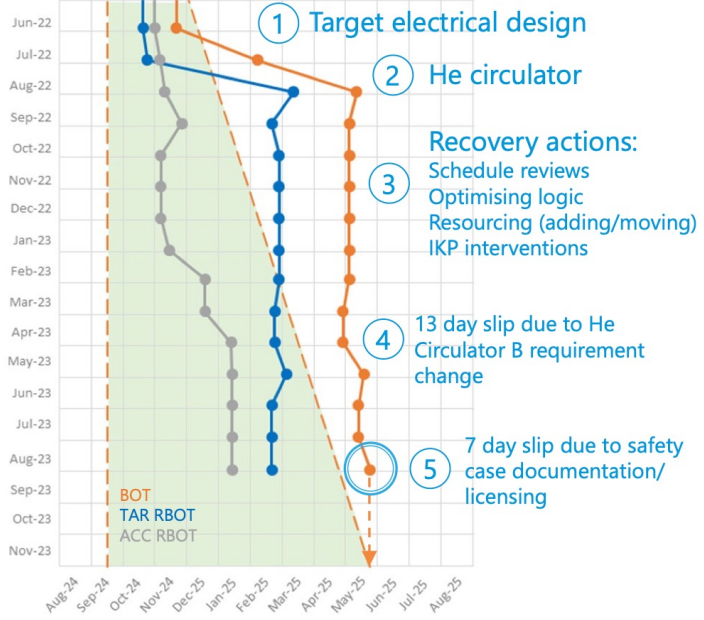




# ESS & Science Directorate Update

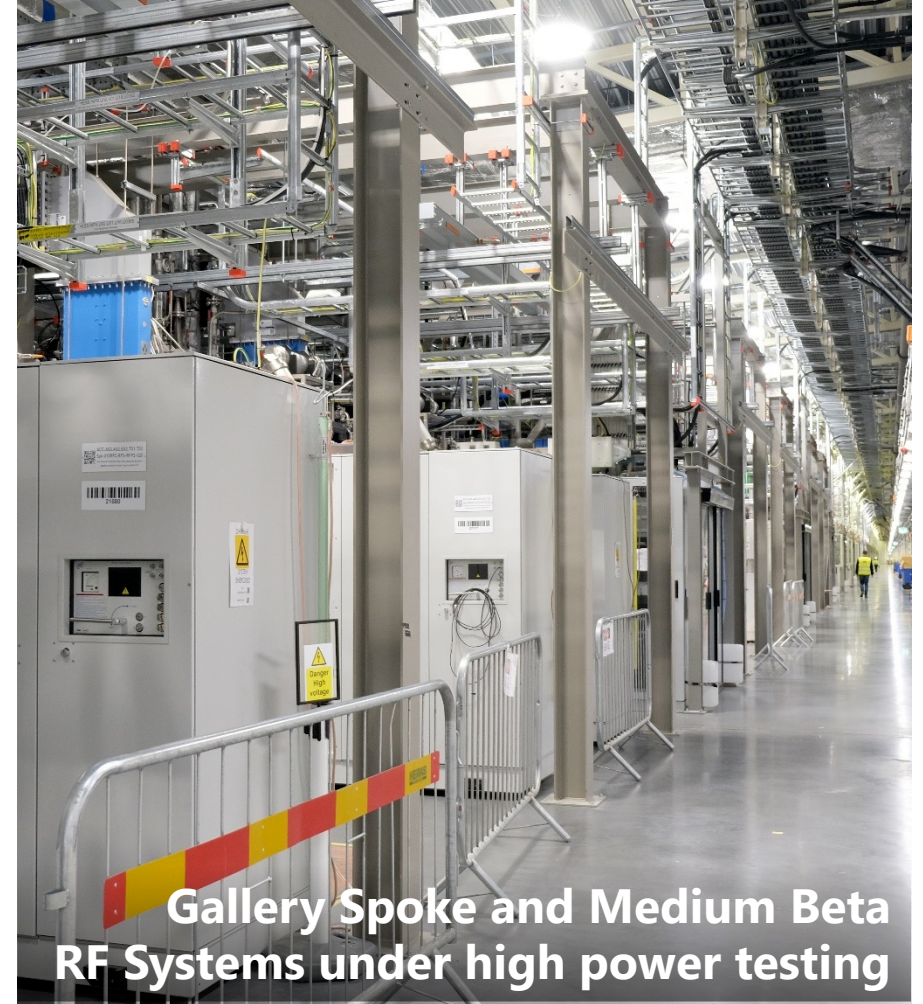
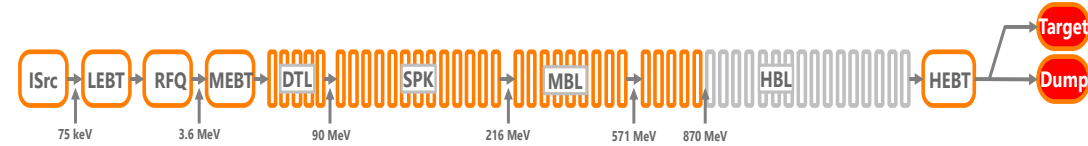
SANS STAP 2023-10-23

# Project Timeline



# Recent achievements

Key activities supported by the whole of ESS



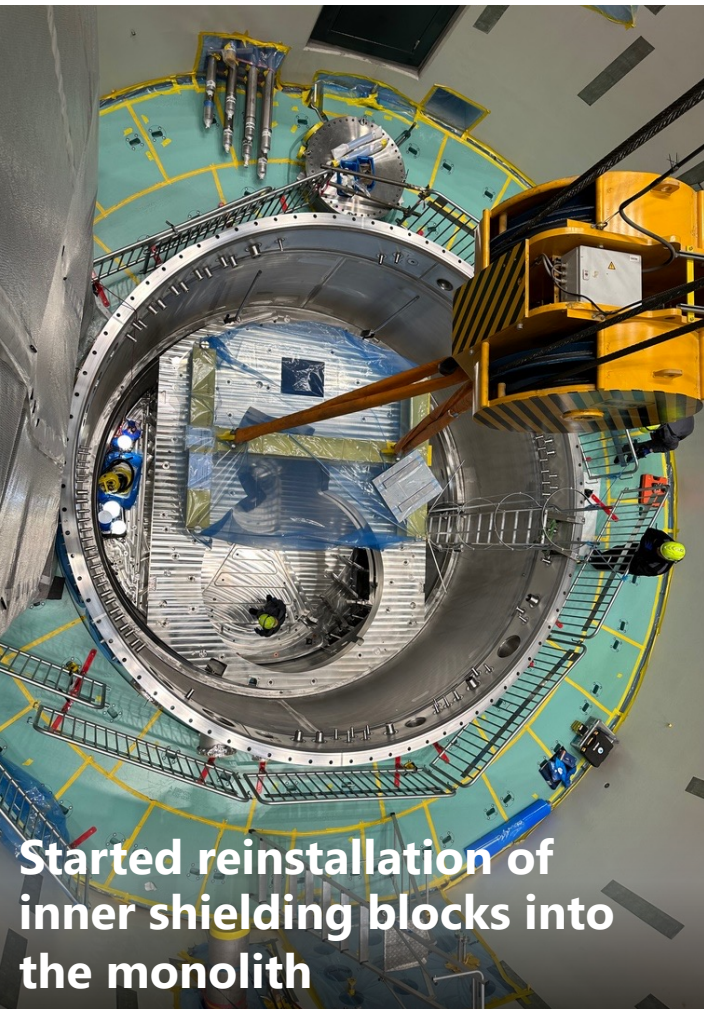
# CDS Cooldown + CM Series Installation

5 SPK + 1 ELL CMs now in the tunnel

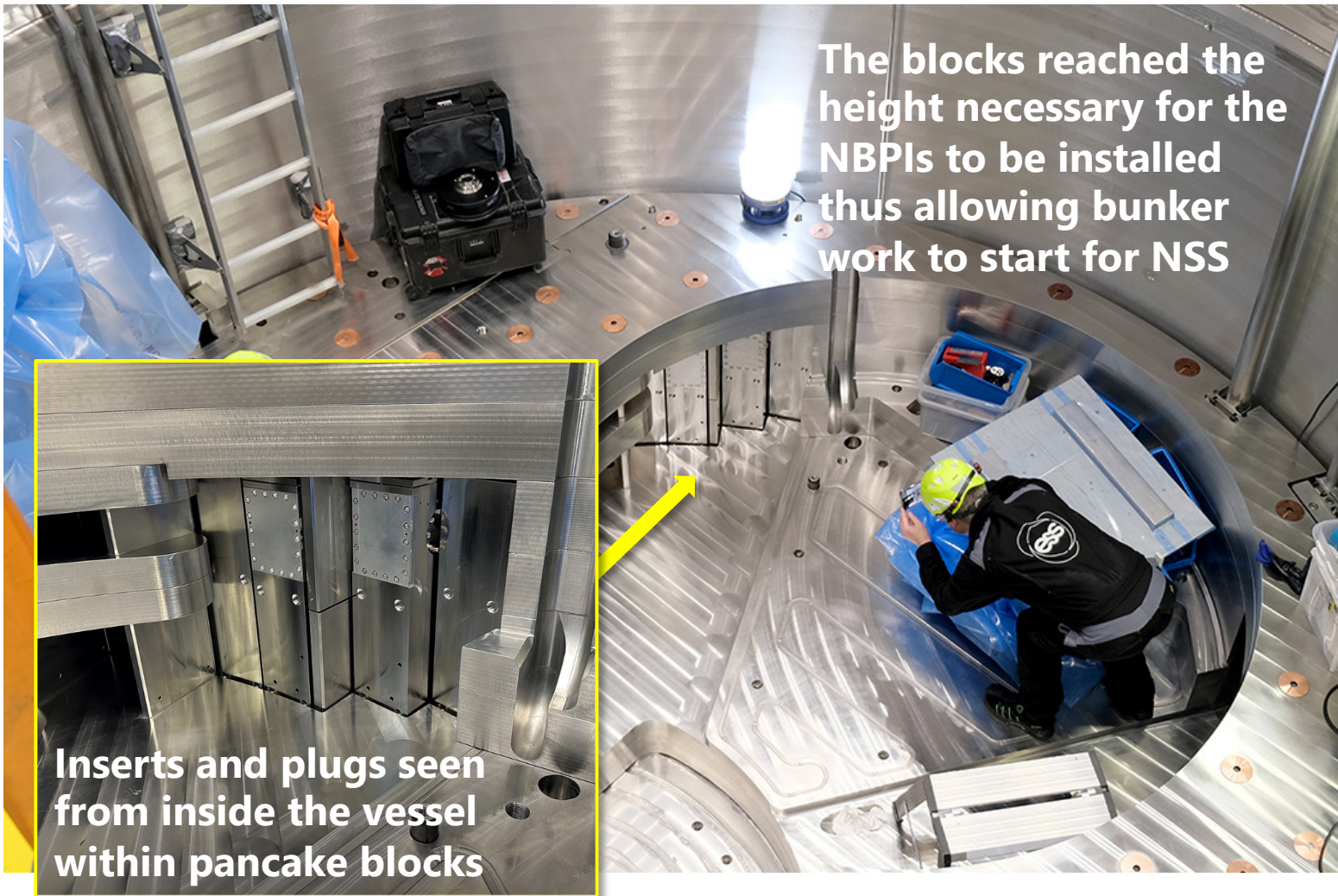


# Recent achievements

## Key activities and progress



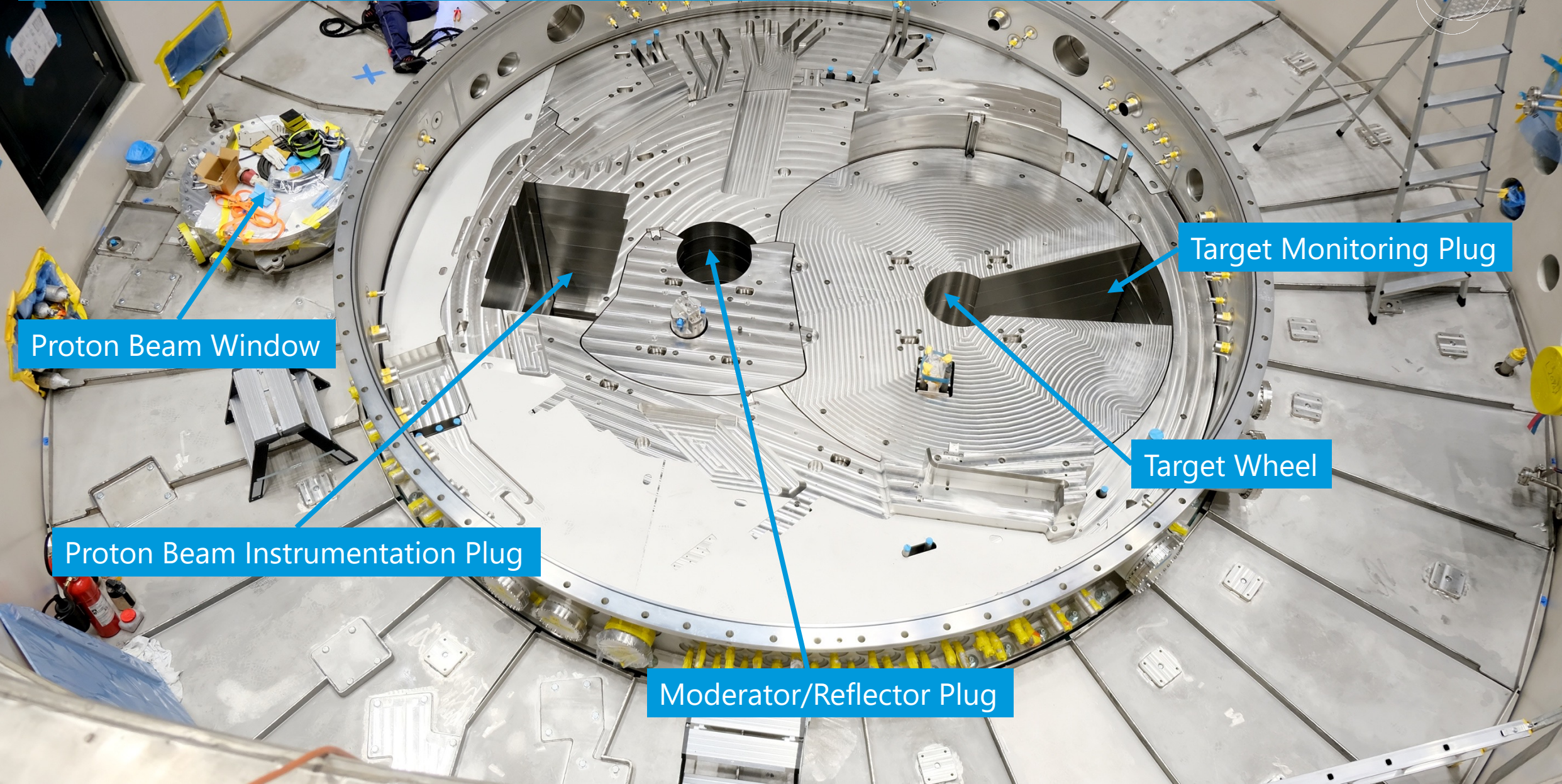
**Started reinstallation of inner shielding blocks into the monolith**



**The blocks reached the height necessary for the NBPIs to be installed thus allowing bunker work to start for NSS**

**Inserts and plugs seen from inside the vessel within pancake blocks**

# Shielding completed



Proton Beam Window

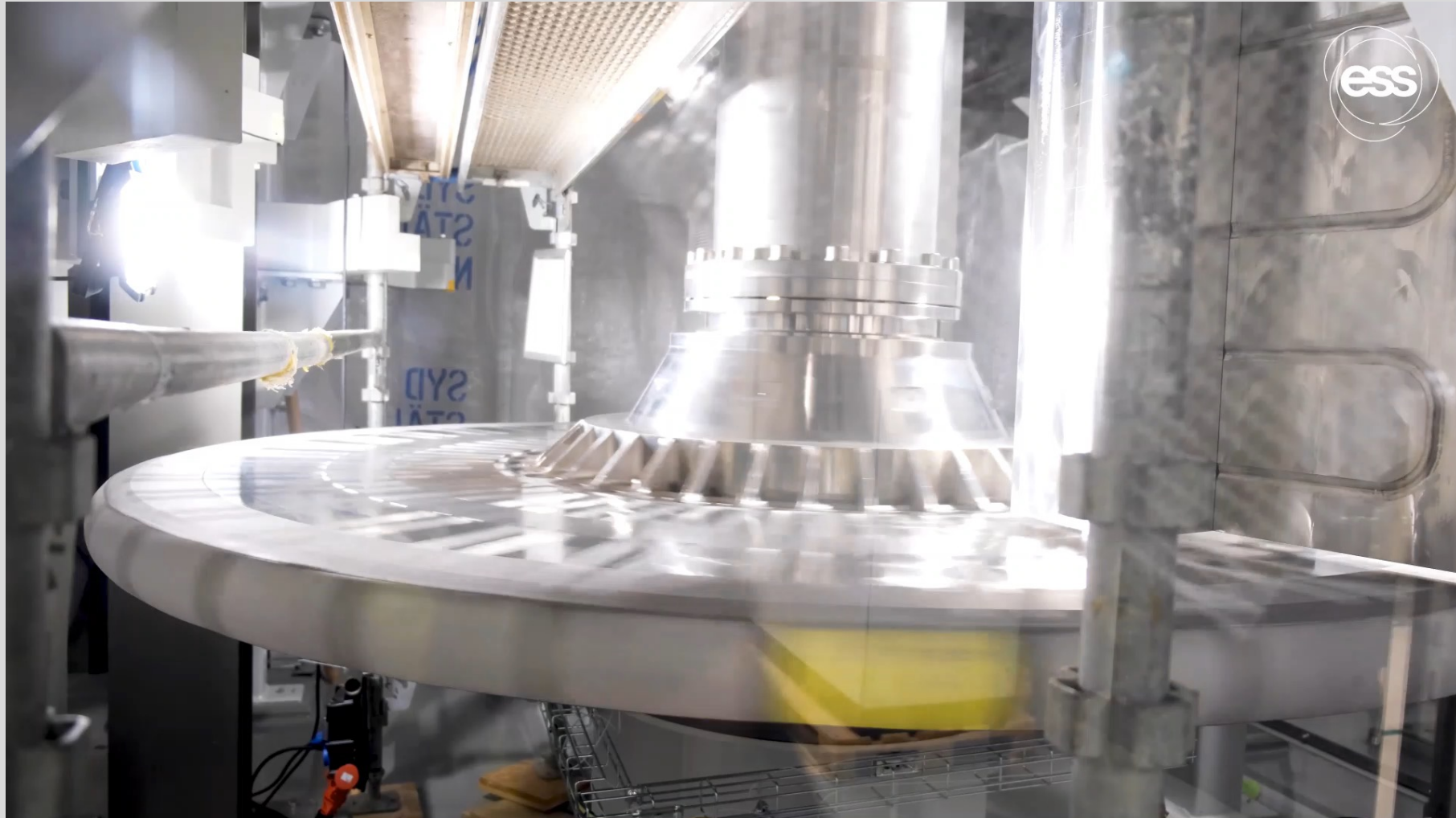
Proton Beam Instrumentation Plug

Moderator/Reflector Plug

Target Monitoring Plug

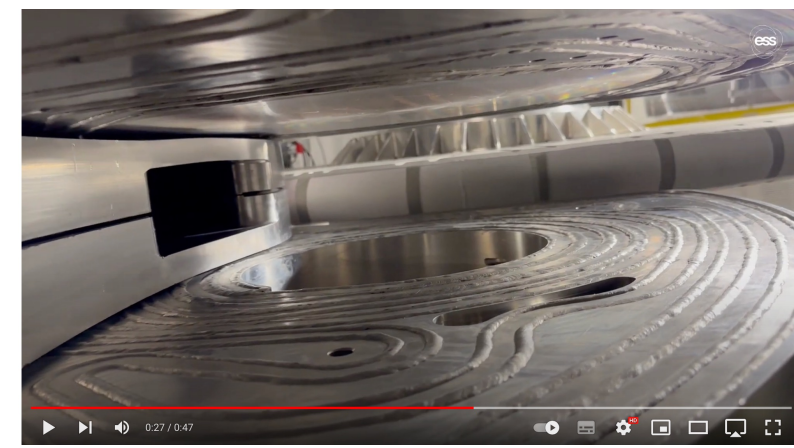
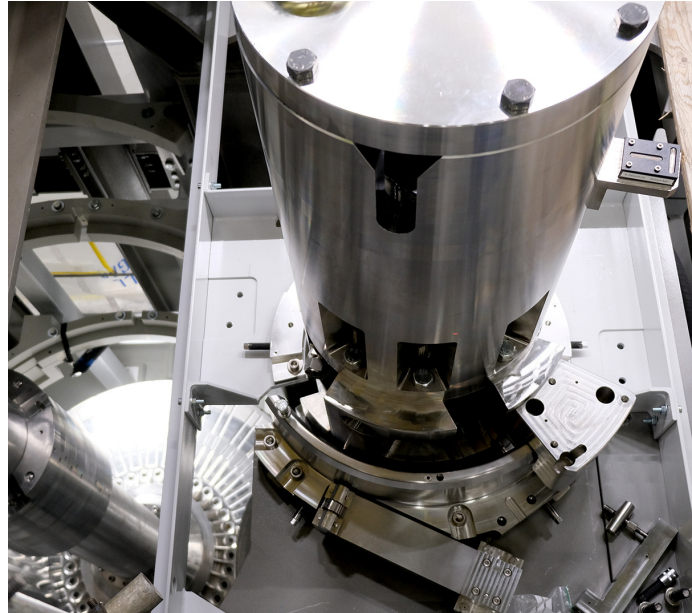
Target Wheel

6 weeks test wheel rotation happening now!



# Recent achievements

## Key activities and progress



Moderator installation in the MUTS and subsequent cleaning of the external and internal surfaces.

Now it is inside a temporary cleanroom next to the MUTS, pending further cleaning/quality improvements.



Installation of inserts and plugs is progressing well, the south sector is complete. Next up is the east sector.



# Light Shutter System

ess

All NBPI and windows installed and vacuum test successful!  
First light shutter system installed



*Some news from the directorate...*

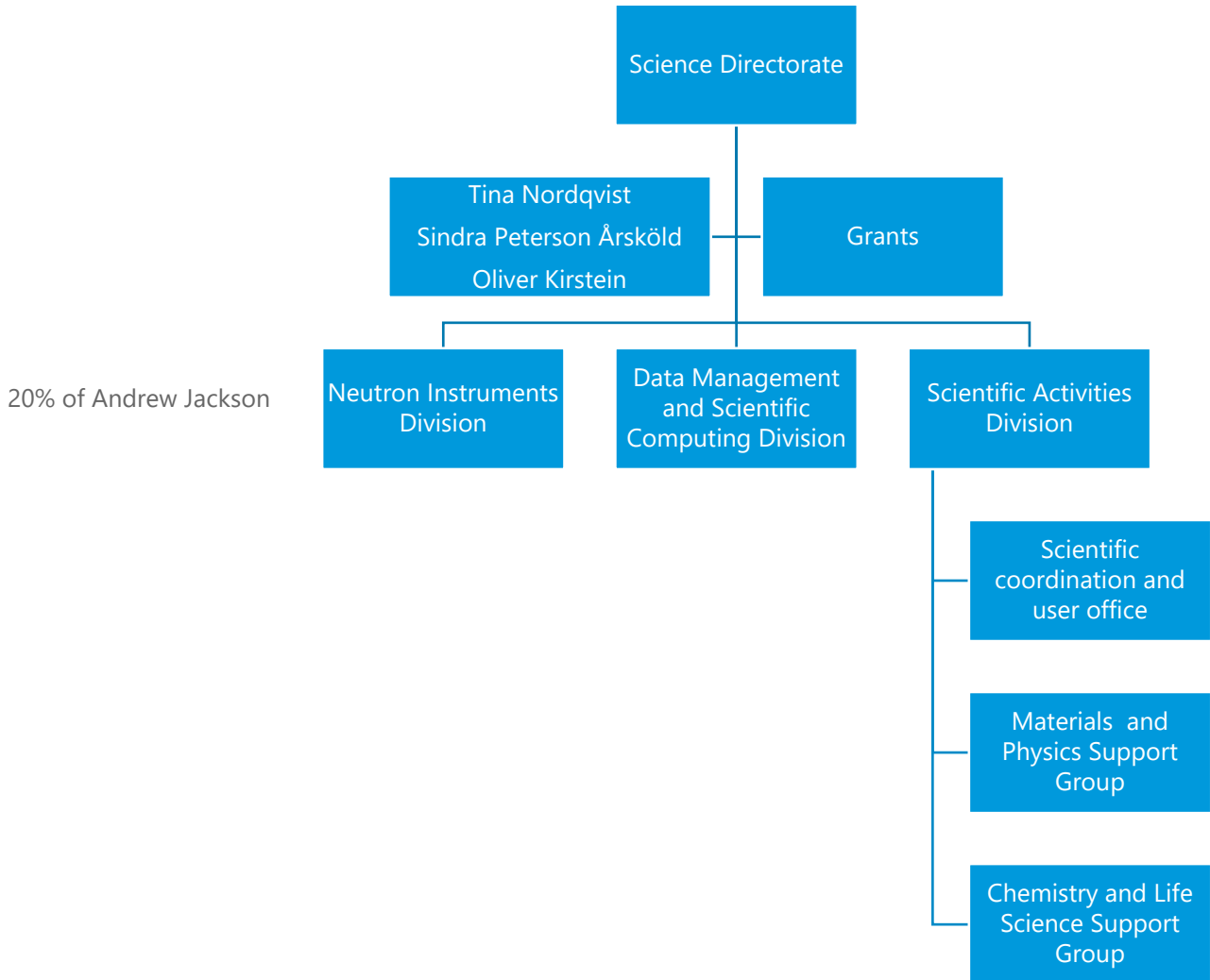
*Implementing changes to get ready for delivering neutron science:*

- structure of directorate*
- benchmarking instruments*
- plans for user involvement*



# Current organizational chart – Science Directorate

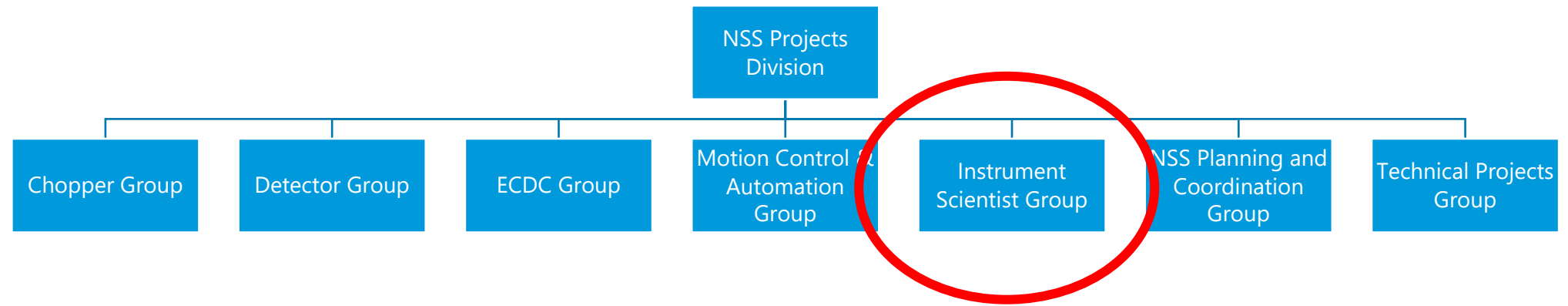
The organisational chart, as it looks now





# Current organizational chart – Technical Directorate, NSS Projects Division

The organisational chart, as it looks now





# New organisation from January 2024

A stronger science management structure, a more efficient way to carry out scientific activities, a stronger voice for science in the ESS organisation.

It is planned to eliminate the NID division in the Science Directorate and replace it with three instrument divisions where instrument class scientific support will be associated. They will be:

- **Large Scale Structure** Division (personnel affiliated to Loki, Skadi, Estia, Freia, NMX)
- **Spectroscopy** Division (personnel affiliated to BIFROST, C-SPEC, Miracles, T-REX, Vespa)
- **Diffraction and Imaging** Division (personnel affiliated to Dream, Magic, Odin, Heimdal, Beer, TBL)

It is also planned create a **Research Coordination Office** group regrouping SCUO, library, communication and grants activities

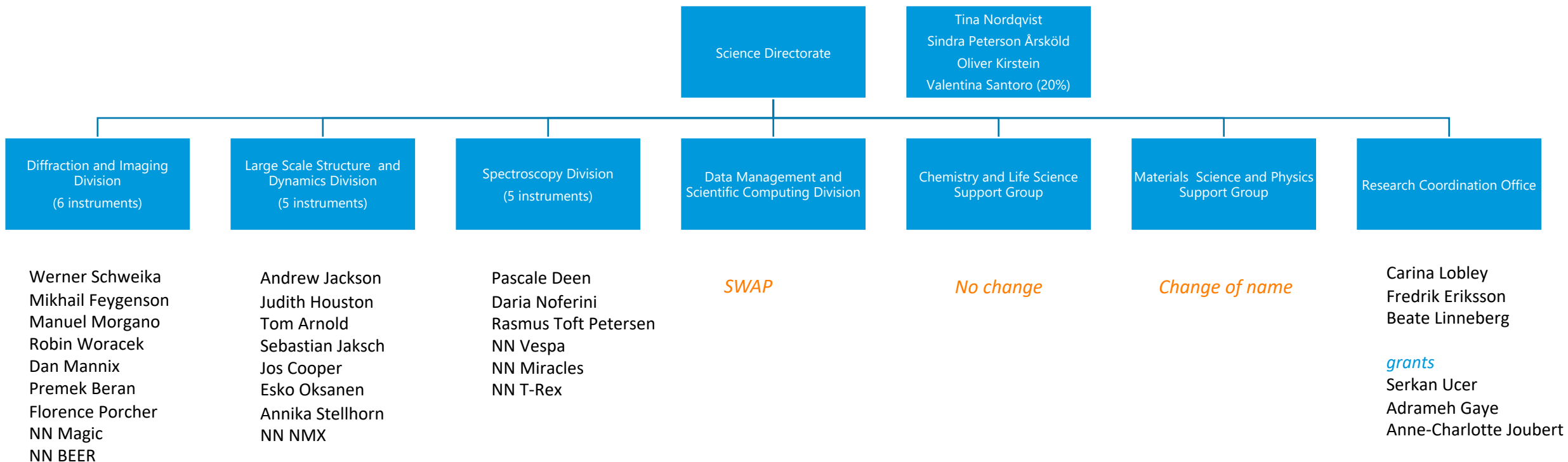
# New organizational chart – Science Directorate

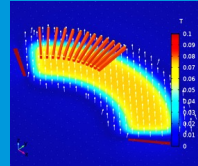
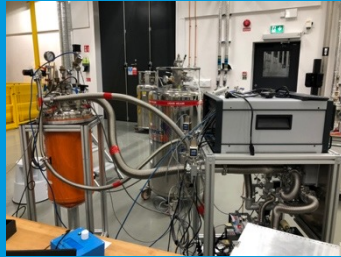
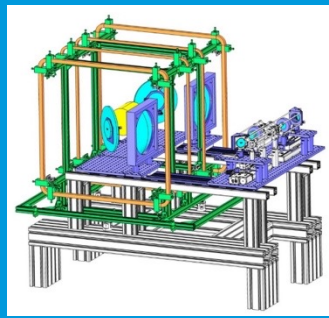


The organisational chart, as it will look from January 2024

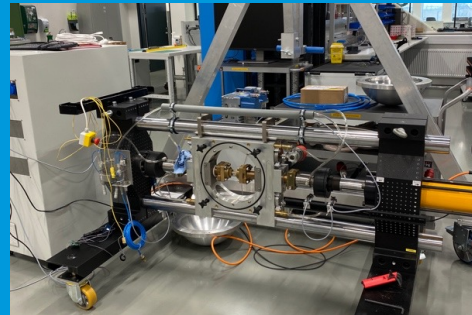
Please note that the size of the three instrument divisions will increase largely in 2024 and it is important that the new divisions' heads participate to the hiring of new scientists.

Head of DMSC – interviews completed  
 Heads of new divisions and group – selection in progress





# Sample environment & support laboratories



## Materials and Physics Support

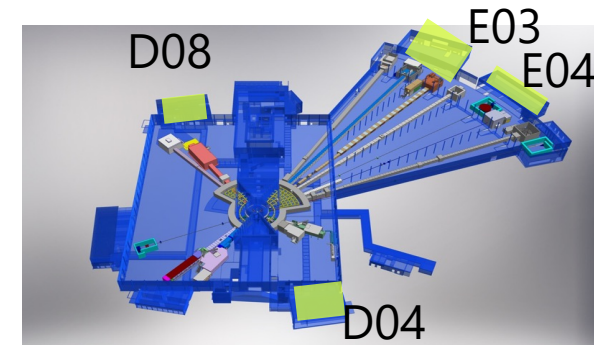
### The MPS scope:

- Provide sample environment systems and users support for low and high temperatures, magnetic and electrical fields, high-pressure and mechanical constraints, **polarisation**.
- Provide SES control integration of complex systems and mechanical integration

## Chemistry and Life Science Support

### The CLS scope:

- Support laboratories (Installation/Spallation Chemistry)
- Sample environment for chemistry and soft matter
- Deuteration service
- Interaction Science





# Scientific Coordination and User Office



Ensuring administrative support for science division activities


ESS successfully hosted a booth with the ILL at ECNS 2023



A collaboration between ESS and our neighbouring universities have won the bid to host ICNS 2025 in Copenhagen and Lund

SCUO are working with IT to implement an e-library to provide journal access for ESS scientists

A recently hired librarian will drive this work



User access policy to be validated at next Council



## Move to DTU in March 2024

Loss of personnel puts in danger hot commissioning  
Location of servers under discussion

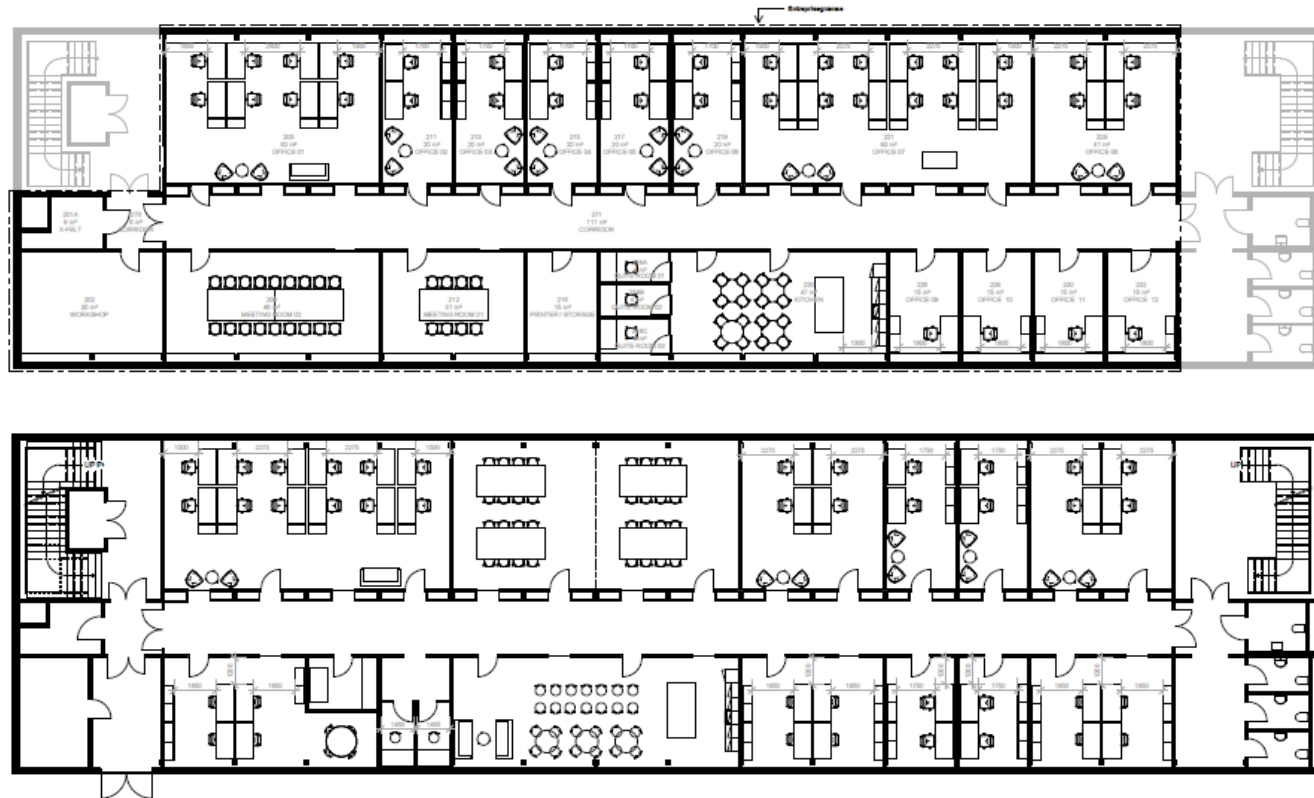


Future office location  
Backup system

Current office location  
Cph data centre (HPC)

Lund data centre  
Support for users, instruments, & Science

# Floorplans



Renovation of 2<sup>nd</sup> floor  
finished 15<sup>th</sup> of February 2024

Renovation of 1<sup>st</sup> floor finished  
ultimo 2024

Option for opening kitchens to  
the hallway and internal  
staircase (TBD 2025)



# Staffing and competence

Need to build up competences for user support and driving R&D

*1 FTE / instrument – 5 FTEs / instrument div.*

*Current staff:*

- *Céline Durniak (DREAM/MAGIC)*
- *Søren Schmidt (ODIN/BEER)*
- *Gregory Tucker (BIFROST/CSPEC)*
- *Wojciech Potzrebowski (LOKI/SKADI)*
- *Justin Bergmann [PostDoc] (NMX)*

*Two open positions: ESTIA/FREIA & NMX*

Current (and future) staff have expertise in:

- Neutron scattering
- Materials science
- **Data processing, analysis and modelling**
- Software engineering
- Atomistic simulations
- Instrument simulations
- Data Science (ML/AI)
- User Experience (UX)
- Product Ownership (Requirements)
- Scientific collaborations



# ESS instruments & comparisons with world-leading neutron scattering instruments at spallation and reactor facilities.

May 2023

MANUEL MORGANO  
TOM ARNOLD  
JUDITH HOUSTON  
MIKHAIL FEYGENSON  
PASCALE DEEN

ROB BEWLEY  
JACQUES OLLIVIER  
GEORG EHLERS  
ROBERT CUBITT  
LIONEL PORCAR

- Overview of facility upgrades (ISIS, ILL, SNS) - not considering ISIS-II, SNS-2
- Reality for Instruments at ESS & long pulse
- Overview of Figure of Merit (FOM)
- Overview of FOM for instruments in main instrument classes.

# Comparisons



Essential to capture the flexibility of ESS in a realistic and fair manner

Figure of Merit (FOM) varies per instrument class

i.e. Imaging = Flux on sample

Reflectometry = Peak brightness\* divergence  $(v \times h) * \lambda_{\max} / \lambda_{\min}$

Main ESS instrument groups represented by a single instrument,  
comparisons with spallation and reactor source instruments worldwide

Provide

(a) Overview of the expectation in 2016 , Full Scope, 5 MW and compared to relevant current day instruments

(b) Worldwide facility upgrades. Day 1 scope of ESS instruments, ESS 2 MW. (Not considering moderator)

(c) Worldwide facility upgrades. Full scope of ESS instruments, ESS 5 MW.

Instruments comparisons:

Tomography: ODIN compared to NEXT(ILL), ANTARES(FRM2), ICON(PSI), RADEN(J-Parc), IMAT(ISIS).

SANS: LOKI compared to D22(ILL), SANS2D(ISIS), EQSANS(SNS)

Reflectometry: FREIA, ESTIA compared to D17 (ILL), FIGARO(ILL), BLB (SNS), Inter (ISIS)

Diffraction: DREAM compared to WISH(ISIS), POWGEN(SNS) and D20(ILL)

Spectroscopy: CSPEC compared to IN5(ILL), LET(ISIS), CNCS(SNS) and AMATERAS(J-Parc)

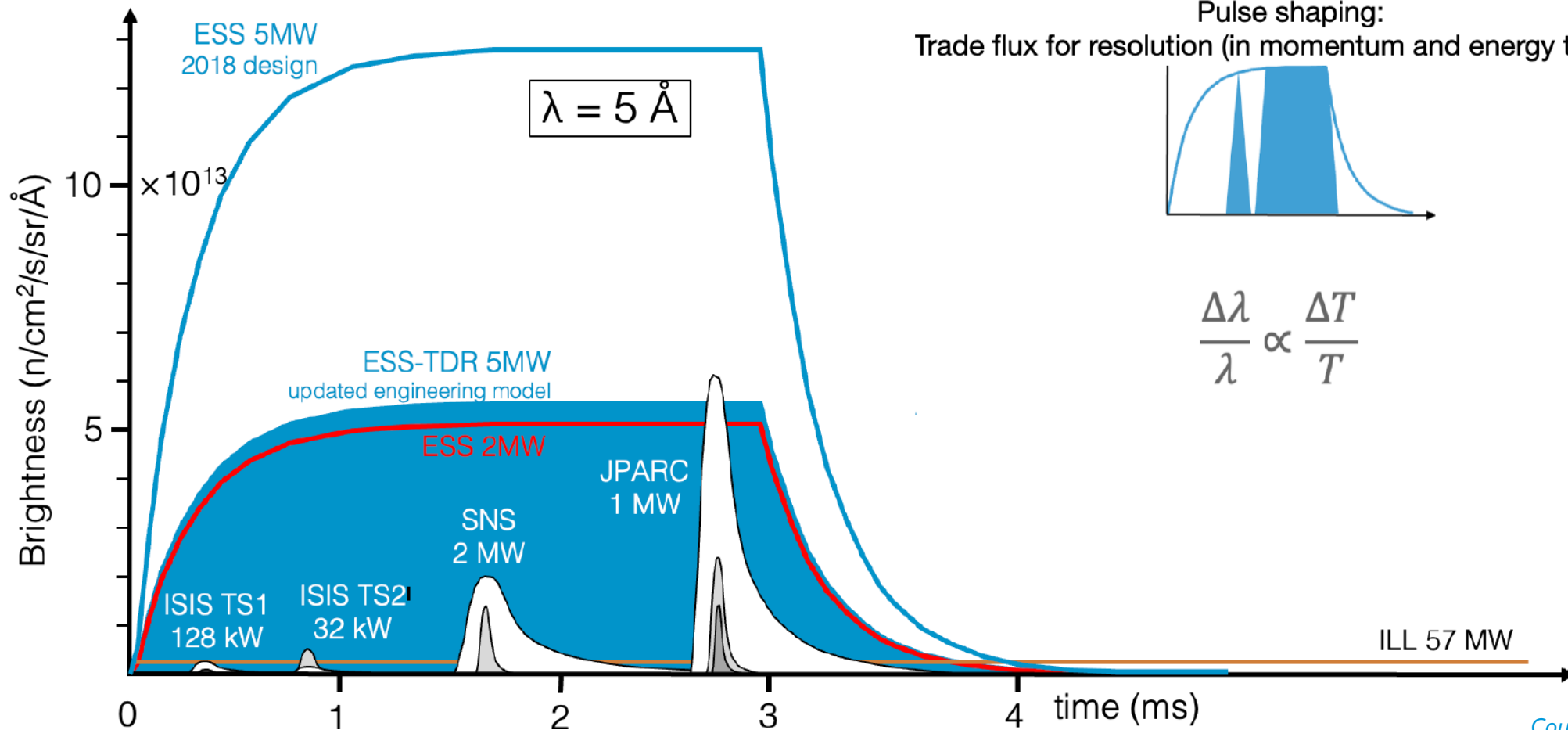
# Capture flexibility of ESS



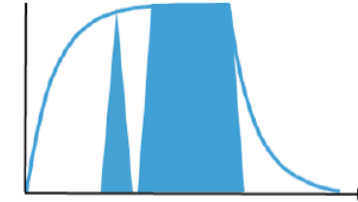
Time averaged brightness of ESS (2 MW) = Time average brightness of ILL

2 MW Relative ESS/ILL peak brightness = 20

5 MW Relative ESS/ILL peak brightness = 50



Pulse shaping:  
Trade flux for resolution (in momentum and energy transfer)



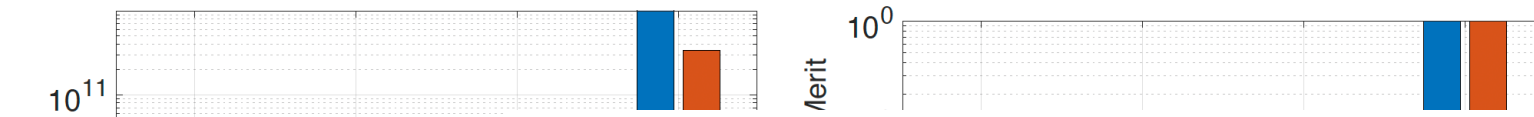
$$\frac{\Delta\lambda}{\lambda} \propto \frac{\Delta T}{T}$$



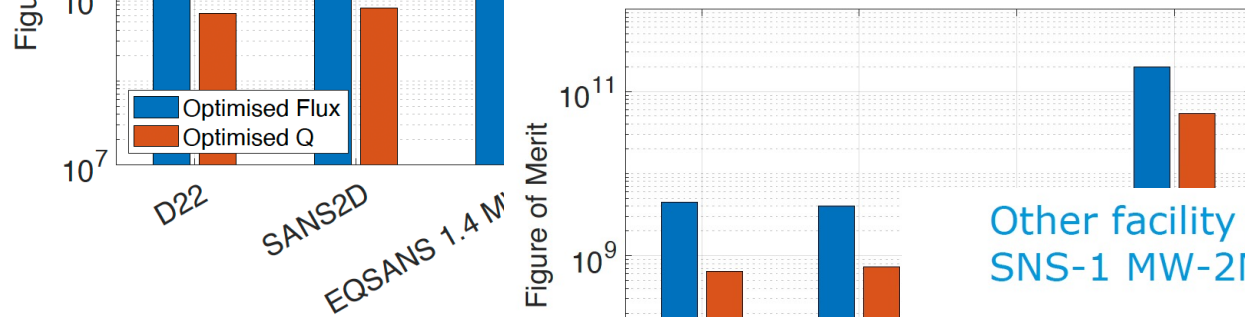


- Tomography
- Reflectometry
- **SANS**
- Diffraction
- TOF Spectroscopy

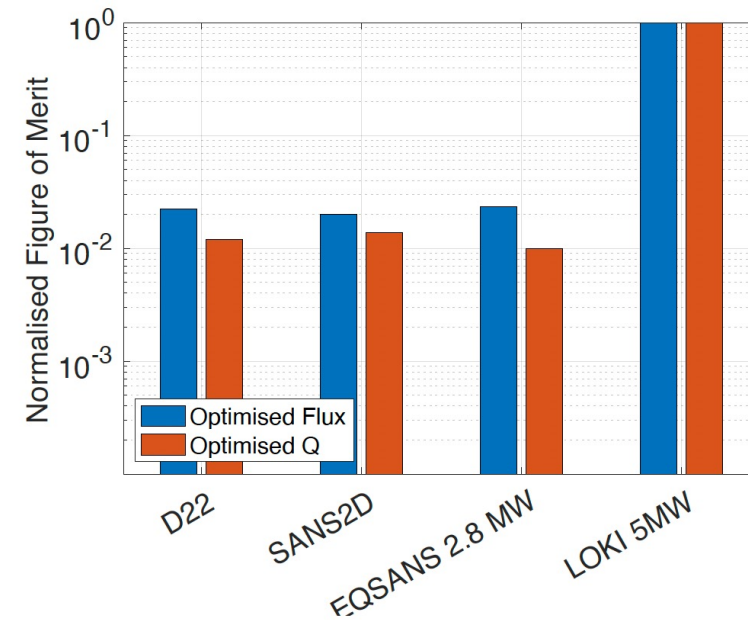
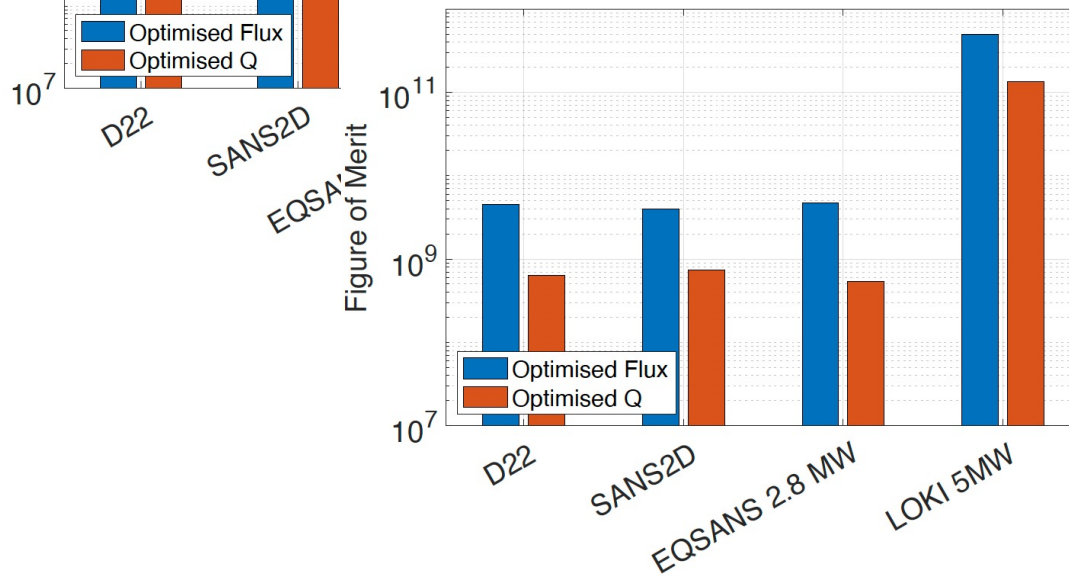
## Expectation in 2016: Full scope & 5 MW



Other facility upgrades:  
SNS-1.4 MW - 2.8MW. ESS-2MW



Other facility upgrades:  
SNS-1 MW-2MW. ESS-5MW





# Setting the expectations

Recent benchmarking with currently upgraded facilities (ILL,SNS, ISIS)

*P. Deen et al.*

- Instruments will be world leading at full scope and 5 MW.
- Many instrument will be best in class at 2 MW and day-1 scope - but will not provide scope for new scientific endeavours: in-operando behaviour, novel states of matter under extreme environments.
- 5MW and full scope will provide access to new scientific domains.
- Note the complementary strength of the ILL instruments.

Rescoping the instruments must become a top priority!

# First/Early Science 'period'

Ideas exist

## Early Science - DREAM

Magnetic nanoparticles, battery materials,...

**Magnetism**

powders  
single-crystals  
nanoparticles  
alloys  
liquids

$Ba_{1-x}K_xFe_2As_2$

weak moments  
phase diagrams of  
superconductors  
multiferroics

orbital ordering  
charge ordering  
distortion  
magnetic exchange

**Energy Materials**

multiphase  
catalysts  
in-operandi  
batteries

**Nanostructures**

many novel samples come in np  
magnetic nanoparticles  
core-shell structures  
self-assembly  
synthesis

**Large Unit Cells**

MOFs  
thermoelectrics  
molecular sieves  
 $H_2$  - storage

## Early Science - LOKI

Taking advantage of q-range, large sample area & low background

Performance @~0.5 MW:  
➤ Comparable(-ish) to SANS2D

**Some current ideas...**

**Photoswitchable worm-like micelles**  
R Evans in Cambridge, UK

System under flow ✓  
Multiple length-scales ✓  
In situ sample irradiation ✓

Requirements: Rheometer integration, lab access

**Amyloid fibril proteins & SEC-SANS**  
I. André, S. Linse in Lund, Sweden

System under flow ✓  
Multiple length-scales ✓  
Bayesian statistics ✓

Requirements: SEC purchase and integration\*, lab access deuterated chemicals, advanced analysis  
\* VR industry grant applied for

**Cyclic fluorescent peptides**  
S Hall in ISIS, UK

Multiple length-scales ✓  
In situ spectroscopy set-up ✓  
Potential to involve ESS DEMAX ✓

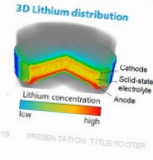
Requirements: NURF integration, lab access, deuterated chemicals

## Early Science - ODIN

Early Science ideas

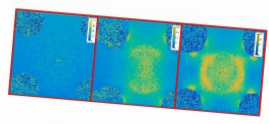
Attenuation tomography / time series (dual mode)

- Battery / battery material
- ANISSA project (ILL-HZB-LU-UM-WWU)
- exchange  $^7Li/^6Li$
- cell development ongoing



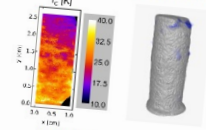
Untextured phase mapping (diffraction contrast)

- Additive Manufacturing / engineering samples
- PSI
- no requirements from SE/Lab/external foreseen



Polarized neutron imaging

- In-situ depolarization analysis of magnets under different conditions
- TUM
- Enabled by in-kind polarization project, SAM involvement



## BIFROST - Early Science Ideas

### Idea 1

**Linewidth studies below 10 meV**  
Showcasing resolution

Phonon linewidth in superconductors drop below  $T_c$ , when gap opens

Phonon linewidths in **thermoelectrics**, SrTiO<sub>3</sub>

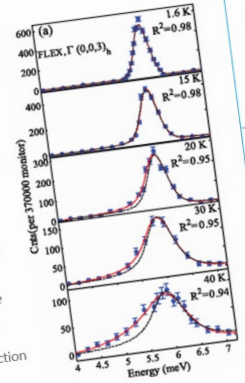
Asymmetric lineshape in magnets, coherence in dimer systems

**Diana Quintero Castro** (Stavanger) Bella Lake / Klaus Habicht (HZB)

**Philippe Bourges** (LLB) Orange cryostat + working software Ongoing grant with Diana @ UIS

Instrument team requirements: Understanding the resolution function well enough to be able

Castro, et al, Phys Rev Lett, (2012)

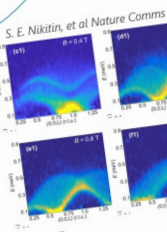
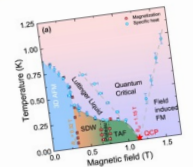


### 'Idea 2'

**Studying underdoped cuprates and cobaltates**  
Showcasing flux at 200 kW

Low energy hourglass excitations are extremely well studied. Most of our target community has some experience with these systems - they can relate.

- Niels Bech Christensen (LLB)
- Johan Chang (Uni Zurich)
- Kim Lefmann (Uni Copenhagen)
- Henrik Rønnow (EPFL)
- Philippe Bourges (LLB)
- Andrew Boothroyd (Oxford)



### Idea 3

**Magnetic excitations in complex phase dia**  
Showcasing mapping efficiency

Showing BIFROST capabilities in applied magnetic field using the Oxford 15 T cryomagnet.

- Ongoing collaborations
- STAPs
- Early Science workshop
- External funding incentives

# ICB satellite meeting

## 12.09.2023

- Several ideas from partners to contribute to hot commissioning and early science with experienced personnel (for secondments we need to solve the VAT issue and clarify the 45 d/y limit for work in SE)
- MoU draft ready – need to start soon negotiations
- Involvement in future workshops
- Help with scientific supervision of “commissioning scientists”/hosting ESS staff at other neutron facilities
- Much interest in possible ESS post-docs...



# Instruments 16-22

*Process to be started*

*GAP analysis to be revisited  
following update of  
instrument benchmarking*

## 2018 CAPABILITY GAP ANALYSIS

The identified two most important missing capabilities in the current instrument suite are:

- **Particle Physics**
- **High-Resolution Neutron Spin-Echo**

An analysis of the remaining capability gaps resulted in the following highlight areas:

- High-Pressure Diffraction
- Grazing-Incidence SANS
- Very Fast Spectroscopy
- Wide Bandwidth Spectroscopy
- High Magnetic Fields

where the first four are new instruments, specialised in areas not adequately covered by the current 15 instruments, and the fifth capability need is for sample environment equipment.

*Activities are going on in Sweden for NPP and GISANS instrumentation*

***Provision of a beam port for HIBEAM under consideration  
Resuming Fundamental and Particle Physics STAP***

# Steady State Operation Review

## 6-8 November 2023

*Proposed STAFF in SD:*

### **INSTRUMENTS**

*FTE/instrument*

3 scientists  
1 instrument associate  
1 post-doc

### **CHEMISTRY & LIFE SCIENCE support**

12 laboratory support  
6 deuteration activities  
5 sample environment  
2 optics support

### **MATERIAL SCIENCE & PHYSICS support**

15 sample environment  
3 polarisation activities

### **RESEARCH COORDINATION OFFICE**

9 FTE (*user office, library,  
industrial liaison, PhD  
programme, research support*)  
3 grant officers

### **DMSC**

60 members of staff as from statutes  
1 data scientist/instrument

### **INSTR. TECHNOLOGY & PROJECTS**

70 FTE (*technical support, choppers,  
detectors, instrument control, projects, ...*)